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Anthony D. Fontanini
Iowa State University

Umesh Vaidya
Iowa State University, ugvaidya@iastate.edu

Alberto Passalacqua
Iowa State University, albertop@iastate.edu

Baskar Ganapathysubramanian
Iowa State University, baskarg@iastate.edu

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Contaminant transport at large Courant numbers using Markov matrices

Anthony D. Fontanini¹, Umesh Vaidya², Alberto Passalacqua¹, and Baskar Ganapathysubramanian⁷¹

¹Department of Mechanical Engineering, 2100 Black Engineering, Iowa State University, Ames, IA 50010, USA

²Department of Electrical and Computer Engineering, 2215 Coover, Iowa State University, Ames, IA 50010, USA

ABSTRACT

Volatile organic compounds, particulate matter, airborne infectious disease, and harmful chemical or biological agents are examples of gaseous and particulate contaminants affecting human health in indoor environments. Fast and accurate methods are needed for detection, predictive transport, and contaminant source identification. Markov matrices have shown promise for these applications. However, current (Lagrangian and flux based) Markov methods are limited to small time steps and steady-flow fields. We extend the application of Markov matrices by developing a methodology based on Eulerian approaches. This allows construction of Markov matrices with time steps corresponding to very large Courant numbers. We generalize this framework for steady and transient flow fields with constant and time varying contaminant sources. We illustrate this methodology using three published flow fields. The Markov methods show excellent agreement with conventional PDE methods and are up to 100 times faster than the PDE methods. These methods show promise for developing real-time evacuation and containment strategies, demand response control and estimation of contaminant fields of potential harmful particulate or gaseous contaminants in the indoor environment.

1. INTRODUCTION

The human body may be exposed to many different types of potential pollutants, pathogens, or chemical and biological agents. These different gases, particulate matter (PM), and illnesses have many different sources. The products of combustion may be lingering in the air from traffic or industrial emissions. Volatile organic compounds (VOCs) may be evaporating or off-gassing from building materials, paints, or cleaning supplies. As people move around the building, dust, mold, pet hair/dander may be suspended in the air. Chemical or biological warfare (CBW) agents may be released during an attack or an act of terror. People coughing or sneezing in office, hospitals, or public transportation vehicles or terminals could be releasing air born infectious diseases into an environment that can affect many people. Some of the health risks related with exposure to these contaminants can be as mild as fatigue, headaches, dizziness, or sinus irritation [1], but could be as severe as aggravated asthma, irregular heartbeat, lung cancer, heart disease, respiratory disease, and in extreme cases can even be fatal [1]. Particulate matter is currently controlled by the National Ambient Air Quality Standards (NAAQS). The particle sizes are generally broken into two classes 1) inhalable particle pollution with diameters < 10 μm (PM₁₀) and 2) fine respirable particle diameters < 2.5 μm (PM₂.₅). Exposure to small diameter PM has been linked to heart disease, lung cancer, cardiovascular and cardiopulmonary diseases [2]. The PM₂.₅ particles are small enough that, when airborne, they experience long suspension times [3], [4], potentially effecting the occupants for long periods of time. The emission of VOCs can have many sources in the indoor environment (paints, adhesives, furnishing, clothing, building materials, combustion materials, and appliances) [5]–[9]. Health effects from VOCs include acute and chronic respiratory problems, neurological toxicity, lung cancer, and throat
irritation [5], [9]–[15]. Gases from the soil or combustion products can also be harmful in large concentrations. Radon, a radioactive gas produced in soils, is the second leading cause of lung cancer [16]. Combustion products (NO₂ and SO₂) from power generation and transportation vehicles can be an asthma aggravate [17], lead to reduced lung function, and reduced lung development in children [18]. These are just some examples of how poor air quality from the surrounding environment, industries, or traffic may affect the human body. For these scenarios, methods for detection, source identification, and real-time estimates of the concentrations can be helpful to keep the concentrations below the recommended exposure limits for the indoor environment.

Other instances where people may be exposed to potentially harmful gases and particulates is during extreme events. These events could be the spread of CBW agents during warfare or an act of terror. In 1995, the Tokyo subway system was attacked with sarin gas [19], which attacks the nervous system. In 2001, Florida, New York City, and Washington D.C. were the sites of anthrax attacks [20]. Other extreme events include the transmission of infectious diseases (TID). In these cases, a small number of individuals carrying an infectious disease enters an often close quarters public area like transportation terminals, public transportation vehicles, schools, offices, and hospitals. Influenza [21] along with the SARS virus [22] has been reported in airports in Asia and around the world. Other highly infectious diseases like measles [23], tuberculosis [24] have been reported in office spaces and hospital wards respectively. In the cases of CBW and TID scenarios immediate detection, fast long-term predictions, planning containment and evacuation strategies, along with identifying the source of the threat may help reduce the overall damage and help save lives.

In order to develop methods and strategies for optimal sensor locations, long-term predictions, determining containment and evacuation in real time, and identifying the sources of the contaminant, a fast and accurate contaminant transport method is needed. There are three broad approaches to construct spatial distribution of contaminants within a building zone: the partial differential equation (PDE) method, the Lagrangian method, and the Markov method. For each of these methods, the starting point is the underlying flow field, calculated by computational fluid dynamics (CFD) or experimentally by methods like particle imaging velocimetry (PIV). These methods utilize the flow field information to produce a time varying solution of the contaminant concentration in the building zone. The PDE method is the most common one used in literature [25]–[29], where the advection diffusion equation PDE is solved on the underlying flow field. For particle transport, Lagrangian methods are popular [27], [30]–[34]. More recently, Markov methods have been developed [4], [27], [35]–[37] which use Markov/transition matrices to propagate the scalar concentrations. Each of these methods have been shown to accurately describe the process of scalar or particle transport in and around buildings.

Although the PDE and Lagrangian methods are older and more established, the Markov method has some distinct advantages. First, the Markov matrix encodes all potential contaminant transport via the transition matrix formulation [36]. This information has shown to be very helpful in calculating optimal sensor locations [38], which places sensors in locations where contaminants naturally collect. This information may also be helpful for real-time contaminant source location identification and calculating sensor estimators for estimating contaminant transport in buildings. Second, the Markov method has been shown to be faster than the PDE method, and in some cases faster than the Lagrangian methods [27], [36]. Markov matrices have also been used to quantify mechanical ventilation performance [39] by using the fundamental matrix of absorbing Markov chains. Although these advantages have shown promise to the applicability of Markov methods, a major limitation has been the construction of the Markov matrices themselves. Markov (or transition) matrices are typically constructed from the flow field by advecting Markov cells and identifying their transition probabilities [36]. The first methods used to calculate Markov matrices came from multi-zone methods [35], [37] which are flux based methodologies. In the flux based methodology, as the time step associated with the Markov matrix increases beyond a Courant number of 1.0, the transition probabilities in the Markov matrix become progressively inaccurate [27]. To resolve this issue, we recently developed a set-based method with Lagrangian particle dynamics which allowed using
larger time steps [36]. While conceptually resolving the time step limitation, this approach required accurate tracking of (potentially) highly deformed sets with associated computational geometry challenges, especially for very large time steps. Furthermore, previous construction (and deployment) of Markov methods have only been shown for steady-state flow fields. Resolving these limitations are the motivation for the current work. The overarching objectives of this paper are to establish methods for calculating accurate and usable large Courant number Markov matrices, and extend Markov matrix based transport analysis to transient flow fields.

We first discuss two different methods for calculating large Courant number Markov matrices. The first method uses multi-step matrices, while the second method uses an Eulerian method to calculate individual rows of the Markov matrix. Calculation of time varying source terms at large matrices is then discussed. Calculating contaminant transport in a time varying flow field using Markov matrices is next shown. Speed increases seen by using the Markov method versus the PDE method is explored. For broader use by the community, methods for constructing the Markov matrices are implemented in an open source CFD framework OpenFOAM [40]. The methods developed in this paper allow for long-term predictions of the movement of contaminants to be made very quickly, optimal sensor locations (using the algorithm in our previous work [38]) for transient flow fields to be determined, and may lead to better utilization for HVAC demand response control of contaminants in the indoor environment.

The outline of this paper is as follows: Methods for simulating contaminant transport in steady and time varying flow fields using Markov matrices is discussed in section 2.1 and the calculation of large Courant number time varying source terms is presented section 2.2 and section 2.3. Next, the benchmark problems used in the analysis are discussed in section 2.4, and validation is shown in section 2.5. Then results are shown for contaminant transport for large Courant number steady-state flow fields in section 3.1, time varying source terms under a steady flow field in section 3.2, and time varying flow fields are shown using the example problems in section 3.3. The computational time is compared between the PDE method and the Markov method shown in this work in section 3.4. Finally, the applicability and implications of these methods are discussed in section 4 and we conclude in section 5.

2. METHODS

This section first provides a quick overview of how Markov matrices can be used for contaminant transport in steady and time varying flow fields. Then we detail the two methods for computing the Markov matrices under large Courant number conditions. Finally, the method for calculating the time varying source terms in the Markov analysis is discussed.

2.1 Continuous and discrete representation of contaminant transport

The well-known advection-diffusion PDE, Eq. 1, for contaminant (scalar) transport is given as

$$\frac{\partial \phi}{\partial t} + \nabla \cdot (U\phi) + \nabla^2(D\phi) = S$$

(1)

The advection-diffusion equation describes the temporal evolution of a continuous scalar field transported by a continuous vector field with sources. The source term, $S$, is a combination of both sources from an inlet and a volumetric source. The velocity field can be either time varying (transient), $U_t$, or time invariant (steady state), $U$. In order to numerically solve this equation, the equation is typically discretized, both spatially and temporally. Spatially, the equation is solved on a domain $\Omega$ composed of a set of cells $\omega = \{\omega_1, ..., \omega_n\} \in \Omega$ and a set of boundary patches, $\Gamma = \{\Gamma_1, \Gamma_2, ..., \Gamma_{nb}\}$, composed of inlets, $\Gamma_{in} \subset \Gamma$, walls $\Gamma_w \subset \Gamma$, and outlets, $\Gamma_{out} \subset \Gamma$. Temporally, the time interval of interest, $\tau$, is discretized into a set of discrete time instances, $t = \{t(0), t(1), ..., t(m)\}$ with $t(0) < t(1) < t(2) < \cdots < t(m)$ and corresponding time steps, $\Delta t_{i+1} = t_{i+1} - t_i$. The scalar concentration evolution is simulated for a set of flow field snapshots
\[ \mathbf{U}_t = \{ \mathbf{U}(0), \mathbf{U}(1), \ldots, \mathbf{U}(m) \} \]. In an abstract setting, the numerical scheme used to solve Eq. 1 in the domain from a given time instance to the next time instant creates a mapping, \( L(\cdot) \), Eq. 2.

\[ \phi_{(i+1)} = L(\phi_{(i)}) \]  

(2)

This mapping for the advection-diffusion equation is a generalization of the continuous version of the Perron-Frobenius (PF) operator [41]. The discrete version of the PF operator (also called the Markov matrix, \( \mathbf{P} \)) is given in Eq. 3, and is used to map the discretized contaminant field from one time step to the next. Note that this is done via simple matrix-vector product, thus providing enormous computational advantages.

\[ \psi_{(i+1)} = \psi_{(i)} \mathbf{P} + \mathbf{S}_{(i,i+1)} \quad \text{for} \quad i = 0: (m - 1) \]  

(3)

The discrete analog of the scalar field, \( \psi_{(i)} = \{ \psi_{(i)}(1), \psi_{(i)}(2), \ldots, \psi_{(i)}(n) \} \) at a given time, \( t_{(i)} \) is the cell volumetric averages of \( \phi \) given by

\[ \psi_{(i)}(k) = \frac{1}{V_{ok} \int \int \int_{Vok} \phi(x,y,z,t_{(i)}) \, dV} \quad k = 1, \ldots, n \]  

(4)

For a constant flow field, a single matrix \( \mathbf{P} \) with an associated time step calculated from the flow field snapshot, can be used to evolve the scalar field. The matrix \( \mathbf{P} \) is a square probability matrix, Eq. 5, with all non-negative entries called transition probabilities.\(^1\)

\[ \mathbf{P} = P(i,j) = \begin{bmatrix} P_{11} & P_{12} & \cdots & P_{1n} \\ P_{21} & P_{22} & \cdots & P_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ P_{n1} & P_{n2} & \cdots & P_{nm} \end{bmatrix} \]  

(5)

For time varying flow fields, a set of flow field snapshots, \( \mathbf{U}_t \), contains the information to evolve the discrete cell concentrations for the time interval of interest. In this case, a set of Markov matrices are constructed, one Markov matrix, for each snapshot \( \mathbf{U}_{(k)} \). These matrices, Eq. 6, are used to evolve the scalar field for each time instant in \( t \), Eq. 7(a-c).

\[ \mathbf{P}(t) = \{ \mathbf{P}_{(0,1)}, \mathbf{P}_{(1,2)}, \ldots, \mathbf{P}_{(m-1,m)} \} \]  

(6)

\[ \psi_{(1)} = \psi_{(0)} \mathbf{P}_{(0,1)} + \mathbf{S}_{(0,1)} \]  

(7a)

\[ \psi_{(2)} = \psi_{(1)} \mathbf{P}_{(1,2)} + \mathbf{S}_{(1,2)} \]  

(7b)

\[ \psi_{(m)} = \psi_{(m-1)} \mathbf{P}_{(m-1,m)} + \mathbf{S}_{(m-1,m)} \]  

(7c)

As discussed earlier, the advantages of using Markov matrices is in the computational speed of propagating the scalar once the matrix has been calculated [3], [27], [36]. Additional advantages include simple identification of optimal sensor locations [38], as well as to compute estimates of the performance of mechanical system air distribution [39]. A major limitation to previous developed flux-based methods for construction of Markov matrices is the small time steps (\( \text{Co} \sim 1.0 \)). The flux based methods start to break down because the entries of \( \mathbf{P} \) are calculated only for neighbors of any given cell, \( \omega_i \). Therefore, for larger time steps, with \( \text{Co} > 1.0 \), the transitional probabilities become increasingly more inaccurate. These effects might be limited to small regions of the domain at first, but over long time intervals of interest or long time

\(^1\) The Markov matrix has other properties that are explained in our previous work [36, 38, 39].
steps these errors can dominate the results [27].

Figure 1 shows a 1D graphical example of how the flux-based calculation methods can break down for large Courant numbers. Each of the 4 states are the same size, $dx$, and in each state the air velocity is the same. Therefore, there is an air flow rate between each adjacent states, $Q(i, i+1)$. If a passive scalar is advected for a Courant number, $Co = 0.5$ (the small dashed state in Figure 1), the flux based methods work well. The transition probabilities for state 0 would be $P(0,0) = 0.5$, and $P(0,1) = 0.5$. The scalar only transitions to the adjacent state, state 1, and not state 2 or state 3. On the other hand, if a passive scalar is advected for a large Courant number, $Co = 2.5$ (the large dashed state in Figure 1), the flux based methods to not work well. The transition probabilities for state 0 should be $P(0,2) = 0.5$, and $P(0,3) = 0.5$, while the flux based method produces an incorrect result of $P(0,1) = 1.0$. The flux-based method restrict the scalar from propagating further within the time step, because only first-order neighbors are stored in the mesh connectivity information. To overcome this limitation two options are available: 1) calculate and use multi-step transition probabilities from a smaller time step to propagate the scalar further in time with a single Markov matrix, 2) use a non-flux based method (like the Eulerian technique explained in section 2.3) to calculate the transitional probabilities for a larger time step. We explore both options in the remaining part of the paper.

![Figure 1: Graphical representation of the breakdown of the flux based methodology for large Courant numbers. The smaller dashed state is state 0 advected by a $Co = 0.5$, and the larger dashed state is state 0 advected by a $Co = 2.5$.](image)

2.2 Calculating multi-step Markov Matrices

The first approach for calculation large Courant number Markov matrices uses the multi-step transition probability feature of Markov matrices. This technique can be used for both steady and transient flow fields. For steady state flow field problems, calculation of the multi-step transition probability equations takes the form of Eq. 8(a-c).

$$\Psi_{(1)} = \Psi_{(0)} P + S_{(0,1)} \quad (8a)$$

$$\Psi_{(2)} = \Psi_{(0)} P^2 + (S_{(0,1)} P + S_{(1,2)}) = \Psi_{(0)} P_{(0,2)} + \tilde{S}_{(0,2)} \quad (8b)$$

$$\Psi_{(m)} = \Psi_{(0)} P^m + (\sum_{i=0}^{m-1} S_{(m-i-1,m-i-0)} P^i) = \Psi_{(0)} P_{(0,m)} + \tilde{S}_{(0,m)} \quad (8c)$$

This strategy for steady flow fields involves taking $m$ matrix-matrix products of the Markov matrix to produce a longer time step associated with the effective Markov matrix, $P_{(0,m)}$. The matrix-matrix multiplication only needs to be performed once and can be done offline and stored in memory, before the transport simulation begins. An effective source term, $\tilde{S}_{(0,m)}$, is constructed, Eq. 8(b-c), since all preceding powers of the Markov matrix would otherwise need to be stored and would eventually result in memory limitations. A method for calculating the effective source terms in the domain offline is discussed in section...
2.4. For transient flow field problems, the multi-step transitional probability equations take the form of Eq. 9(a-c).

\[
\psi_{(1)} = \psi_{(0)} P_{(0,1)} + S_{(0,1)} \tag{9a}
\]

\[
\psi_{(2)} = \psi_{(0)} P_{(0,1)} P_{(1,2)} + (S_{(0,1)} P_{(1,2)} + S_{(1,2)}) = \psi_{(0)} P_{(0,2)} + \tilde{S}_{(0,2)} \tag{9b}
\]

\[
\psi_{(m)} = \psi_{(0)} \prod_{i=0}^{m-1} P_{(i,i+1)} + \left( \sum_{i=0}^{m-1} (S_{(m-i-1,m-i)} \prod_{j=0}^{m-i-1} P_{(m-j-1,m-j)}) \right) = \psi_{(0)} P_{(0,m)} + \tilde{S}_{(0,m)} \tag{9c}
\]

This strategy for transient flow fields shows how to take a set of Markov matrices to construct the effective matrix, \( P_{(0,m)} \), through a set of matrix-matrix products. In the same way as the steady state flow fields, an effective source term can be calculated to reduce memory requirements and decrease calculation time.

2.3 Eulerian method for calculating Markov matrices

Each row, \( i \), of a Markov matrix represents where state \( i \) would transition to in the next Markov time step. The Eulerian method essentially consists of placing a concentration of 1.0 only at state \( i \), Figure 2, and computing how that initial concentration spreads to the rest of the states during the Markov time step, Eq. 10.

\[
P_{(k,k+1)}(i,j) = \psi_{(k+1)}(j) \text{ for } i = 1: n \tag{10}
\]

Notice in Figure 2 that the concentrations are far away from the first-order neighbors of state \( i \) at the next Markov time instant.

![Figure 2: The calculation of a single row \( i \) of the Markov matrix using the Eulerian Markov method. A single state \( i \) is initialized to a value of 1.0, then the advection diffusion equation is solved propagating the cell concentration to other regions in the domain.](image)

This approach calculates the Markov matrix by solving \( n_s \) advection-diffusion equations. Since each row of the Markov matrix can be calculated independently of any other row, all the rows can be simulated in parallel to reduce computational time. Much larger time steps, associated with the Markov matrix, \( \Delta t_{(k,k+1)} \), can be calculated directly without performing the matrix-matrix multiplication in Eq. 8(a-
c) and Eq. 9(a-c). As the number of time steps grows larger, the number of non-zero entries in the Markov matrix increases. To help save memory, at least for shorter time steps, a convenient storage method is using sparse matrices. In sparse matrices only the non-zero entries are stored in a format \( \{i, j, P(i, j)\} \).

2.4 Calculating transient source terms

Contaminant sources can originate at any location in the domain or at an inlet boundary, and the release of the source may take many different forms. The release may be constant, similar to a scenario where smog may be entering a room through an open window, figure 3a. The release may decay exponentially, similar to a scenario where a reaction is taking place in the domain or in the ductwork leading into the domain, figure 3b. The release may be periodic, similar to a situation where a human or animal is exhaling carbon dioxide, figure 3c. Many other release scenarios are possible, where a linear function can be used to approximate smaller intervals of the release, figure 3d. This section discusses a method for calculating the effective source term in Equations 8(c) and 9(c) for both volumetric as well as inlet source terms.

\[
\hat{S} = f(b_0)
\]

\[
\hat{S} = f(b_0e^{b_1t})
\]

\[
\hat{S} = f(b_0\cos(b_1t) + b_2)
\]

\[
\hat{S} = f(b_1t + b_0)
\]

**Figure 3:** Example effective source terms where the source originates from the inlet as a) a constant function, b) an exponential function, c) a periodic function, and d) a linear function.

In calculating the effective source terms, the goal is to provide a generic functional form that can

---

2 For cells with different volumes, the row sum of the Markov matrix may not be 1.0, but the column sum of the Markov matrix should be 1.0. As for uniform discretization of the domain, both the row and column sums should sum to 1.0. Therefore, a uniform discretization results in doubly stochastic matrices, and a non-uniform discretization results in a left stochastic matrix.
easily be calculated offline and easily implemented for online use. The source term in Eq. 1 can be composed of a number of different source terms, $n_{\text{source}} = n_{\text{inlet}} + n_{\text{vol}}$. These sources can either be inlet sources, $n_{\text{inlet}}$, or volumetric sources, $n_{\text{vol}}$, Eq. 11.

$$\tilde{S} = \sum_{i=1}^{n_{\text{inlet}}} s_{i,n} + \sum_{i=1}^{n_{\text{vol}}} s_{i,v}$$  \hspace{1cm} (11)

Each of these sources in Eq. 11 can be collected into a set of contaminant sources that are present in the domain, Eq. 12.

$$\tilde{S} = \{s_{in,1}, s_{in,2}, \ldots, s_{in,n_{inlet}}, s_{vol,1}, s_{vol,2}, \ldots, s_{vol,n_{vol}}\}$$  \hspace{1cm} (12)

We decompose (without any loss of generality) each of these sources into a function of time and space, Eq. 13.

$$\tilde{s}_i(x,t) = g_s(t) f_{s,i}(x) \text{ for } i = 1:n_{\text{source}}$$  \hspace{1cm} (13)

The spatial portion of a given inlet or volumetric source is computed by simulating a unit response of the source over the Markov time step (which is anyway done for the constructing of the Markov matrix). The unit response of the source term, $\tilde{s}_i$, is calculated solving Eq. 1 for the Markov time step and gathering the cell concentrations into a unit response vector for inlet sources \(^3\), Eq. 14, and volumetric sources, Eq. 15.\(^4\)

$$f_{s,i} = \psi(1) \text{ with } \Gamma_{in,i} = g_{s,i}(t)/\max(g_{s,i}(0 \geq t > \Delta t_{(0,1)}))$$ \hspace{1cm} (14)

$$f_{s,i} = \psi(1) \text{ with } \Gamma_{in} = 0, \psi(0)(j) = S(0)/\max(g_{s,i}(0 \geq t > \Delta t_{(0,1)}))$$  \hspace{1cm} (15)

**Remark:** The calculation of the components, $\tilde{s}_i$, of time varying source term, $\tilde{S}$, is similar to using a Green’s function. Since the Markov method is a linear transformation of the contaminant concentrations from one time instant to another, in the same way the spatial unit source vectors can be scaled and superimposed to calculate the time varying effective source term, $\tilde{S}$.

2.5 Test cases and CFD validation

We illustrate developments using three example problems. One case represents a room with a human to measure the influence of displacement ventilation on contaminant transport and source locations for applications in passive smoking and transport of infectious diseases \(^{42}\). The next benchmark case has been used for validating methods for quantifying the performance of ventilation systems and evaluating the effectiveness of the air distribution system in removing contaminants \(^{39},^{43},^{44}\). The final problem is a time varying flow field \(^{38}\) with heated block obstructions and a window (which was used in a previous analysis \(^{38}\)).

2.5.1 Benchmark test for a computer simulated person

The room used in this benchmark test has the following geometric setup, and is shown in figure 3. The room has dimensions of 3.5 (m) x 2.5 (m) x 3.0 (m) in the x, y, and z directions respectively. The inlet (air supply) is positioned in the center of the left wall on the lower edge and has dimensions of 0.4 (m) x 0.2 (m) in the z and y directions respectively. The outlet (air return) is the same dimensions as the inlet, but

\(^3\) If the initial concentration of the inlet source is 0 at $t = 0$, then $\Gamma_{in,i} = g_{s,i}(t)$.

\(^4\) For periodic source terms, it is convenient to use a Markov time step, $\Delta t_{(i,i+1)}$, equal to the period of the source function such that a constant spatial vector, $f_{s,i}$, can be used for the duration of the simulation.
is positioned in the center of the right wall on the edge shared with the ceiling. The benchmark case is manikin free, which allows for different representations of the manikin to be used. Based on the images in the benchmark problem [42], a manikin was created to mimic these images. The manikin was placed 0.05 (m) above the floor in accordance with the benchmark problem to avoid heat transfer between the manikin and the floor. To simplify the computational cost of the simulations, the solution was assumed to be symmetric along the x-axis, which allows for half the room to be modeled. This half of the room and manikin was discretized into 3 different mesh resolutions containing 30,729, 131,431, and 223,637 cells to investigate the convergence of the solution at different mesh resolutions. Figure 4c shows the 223,637 element discretization.

Using the three different discretizations, the simulation of the flow field was performed. The turbulence model chosen for this analysis was the RNG k-epsilon, because of the accuracy shown in previous work [45] on this benchmark problem. Buoyancy effects were introduced using the Boussinesq approximation for density. The inlet air velocity was 0.182 (m/s) at 22 (°C), a turbulence intensity of 30%, and a turbulent length scale of 0.1 (m). This air flow rate gives an air change rate of 0.5 (hr). The manikin generates 76 (W) with 40% convective and 60% radiative heat transfer. While the side walls, ceiling, and floor was designed to be perfectly insulated, some heat transfer was found to have occurred [45]. According to previous work performed on this problem, the heat transfer can be represented as a 10 (W) heat source by the floor [45]. Each mesh discretization and simulation setup was solved to a residual tolerance of $1 \cdot 10^{-4}$ using the “buoyantBoussinesqSimpleFoam” application in OpenFOAM [46]. Once the simulations

![Figure 4: a) The dimensions of the room with the inlet (green) on the lower part of the side wall in front of the manikin and the outlet (red) on the upper part of the side wall behind the manikin. The manikin is positioned in the center of the space. b) The sampling positions along the center of the room where both experimental data and the numerical simulations are compared. c) The discretization of the room and the manikin with 223,637 elements used to create the transition matrices.](image-url)
converged, the air speed and temperature were compared at 4 different positions along the center of the x-axis from the floor to the ceiling, figure 4b.

The results show that there is a small temperature gradient from the floor to the ceiling due to stratification, while a thermal plume is present around the manikin, figure 5a. Results from the 3 different mesh resolutions are shown at each of the sample locations in figure 5. All the different mesh resolutions agree relatively well with the experimental data, figure 6. The sample positions downstream in the manikin L4 and L5 show some discrepancy, but this is mainly due to the fact that the original manikin geometry was not specified by the benchmark problem and that a hoist was used to hold up the manikin during the experiment which may have affected the results. Based on these results the 223,637 element discretization was determined to be an adequate resolution for the rest of the analysis.

Figure 5: a) The air speed surface contours displaying the thermal plume around the manikin and the streamlines showing how air moves around the room. b) The Temperature surface contours showing the air stratification within the room and the thermal plume around the manikin.
Figure 6: a) Air speed comparisons at the sampling profiles between the three different mesh resolutions and the experimental air speed measurements from the benchmark problem. b) Temperature comparisons at the sampling profiles between the three different mesh resolutions and the experimental temperature measurements from the benchmark problem.

2.5.2 Benchmark test for an isothermal room

The room in this benchmark has the following geometry setup and boundary conditions, and is shown in figure 7 and figure 8. The room is 4.2 (m) x 3.0 (m) x 3.6 (m). The inlet is positioned on the near sidewall in figure 7, with dimensions 0.3 (m) along the z-axis and 0.2 (m) along the y-axis. The bottom edge of the inlet is 2.05 (m) from the floor and the center is located along the center xz-plane of the domain. The outlet is also positioned along the xz-plane with dimensions of 0.2 (m) along the z-axis and 0.15 (m) along the x-axis. The inlet air velocity is uniform at 1.68 (m/s). The inlet turbulent kinetic energy is based on a 14% turbulent intensity and the turbulent dissipation rate is calculated from $\varepsilon_{in} = k_{in}^{1.5} / (0.005 \sqrt{A_{in}})$. The air flow field was shown to be relatively symmetric [44], so only half the domain was discretized and simulated.

Figure 7: Dimensions of the benchmark room. The inlet (green) is on the near side wall and the outlet (red) is on the ceiling.
The air in the room was simulated using the RNG k-epsilon model to a residual tolerance of $10^{-6}$ for all solution parameters. These conditions were simulated with two different mesh resolutions (22,680 elements and 181,440 elements). Validation of this numerical model, boundary conditions, and mesh resolutions are shown in our previous work [39]. In our previous work, the age of air, based on passive scalar tracer gas measurements, is compared with experimental values. The results of the simulations of the model, and boundary conditions showed excellent agreement with the experimental values. The resulting flow field of the simulation is shown in figure 8. The results of the simulated benchmark problem show that air travels from the inlet straight across to the far wall. At this point some of the air goes towards the outlet while the rest spreads out along the far wall and is circulated through the rest of the space.

![Figure 8: a) The discretization used in the simulations and the previously validated simulations [39]. The discretization has 22,680 elements. B) The air flow field of the isothermal benchmark problem from the simulated boundary conditions and discretization.](image)

2.5.3 Benchmark test for time varying flow fields

The room in this problem was used in our previous work [38]. The room has the same dimensions as the IEA annex 20 problem [47], with the addition of two obstructions located at 1/3 and 2/3 along the x-axis, figure 8a. These obstructions are heated with 70 (W/m²) and there is a window along the right wall of the room that is heated 100 (W/m²). The inlet temperature is 293 (K), while the rest of the walls are zero gradient. The air enters the room with a Reynolds number of 2,500 until the flow field reaches steady state. Then the air flow rate is doubled to a Reynolds number of 5,000 at $t = 0$ (s). The sudden increase in the air flow rate causes the flow field to be time varying. At $t = 0$ (s), a scalar contaminant is injected into the space from the inlet. All other boundary conditions are consistent with the IEA 20 annex problem [47].
The flow field was solved for using the RNG-k-ε model for turbulence. The domain was discretized into 10,280 elements, figure 9b. This resolution was sufficient to capture the flow field, figure 8c, and the temperature field, figure 9d, during a spatial convergence study. The steady state problem was solved initially to provide the initial conditions of the transient problem. The governing equations for the steady-state problem was solved to a residual tolerance $10^{-7}$ for all solution variables. After the steady-state problem was solved, the Reynolds number was increased to 5,000 and the temporal solution was calculated using a time step of 0.1. This time step with the discretization provided a Courant number of approximately 1.0. Each of the solution variables at each time step was solved to a residual tolerance of $1 \cdot 10^{-6}$.

3. RESULTS

This section shows how the Markov method and PDE methods compare under different flow conditions and source conditions. First, the two methods are compared using a 3D steady flow field with constant source release. In this example, the results show the Markov method using large Courant numbers. The next example shows the results of the Markov based transient source terms for large Courant numbers. Then a set of Markov matrices are calculated and used to propagate the contaminant under a transient flow field. Finally, speed comparisons are made between the PDE approach and the Markov approach for different solving tolerances of the PDE method and Courant numbers for the Markov method. These examples show how the Markov method can be used under steady state and transient flow fields along with constant and time varying contaminant release scenarios.

3.1 Steady flow field contaminant transport

The case simulated to evaluate the Markov methods on a steady flow field at high Courant numbers is the manikin example in section 2.5.1. The advection diffusion PDE was simulated using a gas diffusivity of $7.334 \cdot 10^{-5}$ (m$^2$/s), which represents helium tracer gas in air at 298 (K) [48], and a time step of 0.02-sec which corresponds to a maximum Courant number of 1.0 for the chosen discretization. Three different Markov matrices where calculated with Markov time steps of 0.2-sec, 2.0-sec, and 4.0-sec, respectively, with all three constructed using the 0.02-sec PDE time step. These Markov matrices represent a Courant number of 10, 100, and 200, respectively. The contaminant was released into the domain at a constant rate...
by the inlet at a normalized concentration \((\psi/\psi_{in})\) of 1.0. The contaminant was released in the domain for 1 air change (30 min).

As time progressed, the contaminant starts to fill the room, Figure 10. The concentration of the contaminant initially is advected along the floor and then starts to move its way towards the ceiling. Around the manikin, the thermal plume seen in figure 5a helps carry the contaminant towards the ceiling. The normalized concentration is shown at three different time snap shots at 5-min (figure 10a), 10-min (figure 10b), and 15-min (figure 10c). The concentrations along L1, L2, L4, and L5 of the contaminant at 10-min, 20-min, and 30-min are used to compare the PDE method and the Markov method at different Courant numbers. The results in figure 11 show that for L1, L2, L4, and L5 the Markov method compares very well with the PDE method for the 10-min, 20-min, and 30-min samples. The results of the Markov method are almost overlaid with each other on each of the subplots even at the Courant number of 200. This result shows that the Markov method can be used to take time steps at least two orders of magnitude larger than the PDE method with extremely accurate results.
Figure 10: a) Left: Iso-contours of the normalized contaminant concentration at (a) 5-min, (b) 10-min, (c) 15-min. Right: Normalized contaminant concentrations along the z-centerline plane at (a) 5-min, (b) 10-min, and (c) 15-min.
Figure 11: Comparisons between the PDE method and the Markov method at 10-min, 20-min, and 30-min along the L1, L2, L4, and L5 sample lines.

### 3.2 Time-varying source terms in a steady state flow field

The case used to show how Markov methods perform using transient source terms at high Courant numbers is from section 2.5.2. The gas diffusivity is the same of the previous example. In this problem four different source terms injected from the inlet are analyzed (constant, linear, exponential, and periodic). The four temporal source functions are seen in equations 16a-16d.

\[
\begin{align*}
g_{s,i} &= 1.0 \quad & (16a) \\
g_{s,i} &= \frac{1}{450} t \quad & (16b) \\
g_{s,i} &= e^{-\frac{1}{300} t} \quad & (16c) \\
g_{s,i} &= \frac{1}{2} - \frac{1}{2} \cos\left(\frac{\pi}{5} t\right) \quad & (16d)
\end{align*}
\]

For each of the inlet source functions the effective source terms and Markov matrix was calculated for a Markov time step equal to a Courant number of 16.67, except for the periodic source term in equation 16d where the Markov time step was equal to a Courant number of 166.7. Each of the scalar transport simulations were run for 450 (s).

Snapshots at 210 (sec) and 450 (sec) of the scalar transport simulations can be seen for each source term in figure 12. The concentration of the scalar in the room for the constant and linear source terms cases increases with time in figure 12a-12b and 12c-12d respectively. For the exponential case, the 210 (sec)
snapshot has a higher scalar concentration than the 450 (sec) snapshot, figure 12e-12f. The periodic nature of the inlet source condition can be seen in figure 12g and 12h. At the wall the concentration of the scalar is much higher whereas at the inlet the concentration is much lower. Figure 13 compares the scalar concentrations along the center z-plane at two locations along the x-axis (x = 1.13 (m) and x = 3.2 (m)). Each of the different source terms are compared at three different time instances $t = 150$ (sec), $t = 300$ (sec), and $t = 450$ (sec). For all the inlet source cases (constant, linear, exponential, and periodic) the Markov method and PDE method show excellent agreement. These results show that the Markov method for time varying source terms at high Courant numbers provide the same results as the PDE method at lower Courant numbers.
Figure 12: Results of the transient source simulations with sources at the inlet at a time of 210 (sec) and 450 (sec). a) constant source at 210 (sec), b) constant function at 450 (sec), c) linear function at 210 (sec), d) linear function at 450 (sec), e) exponential function at 210 (sec), f) exponential function at 450 (sec), g) periodic function at 210 (sec), h) periodic function at 450 (sec).
Figure 13: Scalar value comparisons along two lines at the center z-plain at \( x = 1.13 \) (m) and \( x = 3.2 \) (m) between the Markov method and the PDE method for different inlet source functions. a) Constant source function at \( x = 1.13 \) (m), b) linear source function at \( x = 1.13 \) (m), c) exponential source function at \( x = 1.13 \) (m), d) periodic source function at \( x = 1.13 \) (m), d) constant source function at \( x = 3.2 \) (m), b) linear source function at \( x = 3.2 \) (m), c) exponential source function at \( x = 3.2 \) (m), d) periodic source function at \( x = 3.2 \) (m).

3.3 Time-varying flow field contaminant transport

The case used for analyzing contaminant transport in time varying flow fields for both the PDE and Markov methods is from section 2.5.3. The Reynolds number at \( t = 0 \) (s) is increased from 2,500 to 5,000. The transient simulation is run for 400 (s). One hundred Markov matrices are created for the 400 second simulation. Each Markov matrix propagate the scalar over a 4 second horizon, i.e. from \( t = 0 \) (s) to \( t = 4 \) (s), then \( t = 4 \) (s) to \( t = 8 \) (s), ..., \( t = 396 \) (s) to \( t = 400 \) (s). The 4 second time steps for the Markov matrices correspond to a Courant number of approximately 40. Snapshots of the normalized flow field, temperature field, Markov concentrations, and PDE concentrations can be seen at \( t = 132 \) (s), 264 (s), and 400 (s) in figure 14. Figure 14 shows that after the increase in inlet Reynolds number, higher velocity air starts to push back against the buoyancy dominated flow seen in figure 9. A recirculation cell starts to grow, figure 14, as the temperature in the area to the left of the first obstruction cools. Eventually the air jet from the inlet comes down on top of the first obstruction. Meanwhile, the scalar starts to enter the space. Initially the scalar follows the higher speed regions of the space, then starts to diffuse to the centers of circulation. The left side of the room fills first, as most of the air is trapped by the jet landing on top of the obstruction.
Figure 14: Contours of normalized velocity magnitude (top left), temperature (bottom left), contaminant concentrations from the PDE method (top right), and contaminant concentrations from the Markov method (bottom right) for three different time snapshots a) $t = 132$ (sec), b) $t = 264$ (sec), and c) 400 (sec).
Visually there is little difference between the contours of the Markov method and the PDE method at the time snapshots shown in figure 14. Samples from the floor to the ceiling at $x = 1.5$ (m), $x = 4.5$ (m), and $x = 7.5$ (m) are also compared at $t = 132$ (sec), $t = 264$ (sec), and $t = 400$ (sec) in figure 15. For each of the times investigated and all three sampled locations the Markov method provides exactly the same concentrations as the PDE method. These results show that a set of Markov matrices can be used to propagate a contaminant field under a time varying flow field and give equivalent contaminant concentrations as the PDE method.

3.4 Computational time comparisons between the Markov and PDE methods

This section evaluates the computed speed increases by using the Markov method over the PDE method at large Courant numbers along with the memory requirements necessary to store these matrices. For this comparison the 3D problem stated in section 2.5.1 was used to evaluate the speedup using Markov matrices associated with Courant numbers of 10, 100, and 200 from section 3.1. The time required to propagate the scalar from $t = 0$ (min) to $t = 30$ (min) was recorded for the PDE method and the three Markov matrices. For the PDE method, OpenFOAM was used to simulate the PDE method on the steady flow field, and the Markov methods used MATLAB to calculate the scalar propagation. For the Markov method, the operations for each step includes a single matrix-vector product to propagate the scalar forward in time and a single vector-vector addition to add the effective source term at each time step. For the PDE method, the solution tolerance, $\tau$, of the advection-diffusion equation makes a big difference in terms of computational time. As the solution tolerance decreases, more iterations at each time step are needed to solve for the scalar field.

After the simulation times were recorded, the speed increase relative to the PDE method was calculated. Figure 16a shows that for all the solution tolerances and Courant numbers the Markov method
is between 30 and 120 times faster than the PDE method. The increase in speed is mostly due to the use of sparse matrices where only the non-zero entries are stored and require operations during the matrix-vector product. The matrices at least for Courant number \( \leq 200 \) are still very sparse matrices as seen in Figure 16b. The percentage of non-zero entries range between 0.03\% at a Courant number of 10 to 0.4\% at a Courant number of 200. While these percentages may change based on the individual flow field used, they are fairly representative of the sparsity of the resultant matrices. The sparsity percentages should be most sensitive to the Reynolds number or air change rate of the room, the amount of mixing in building zones due to obstructions and people, and the diffusivity of the contaminant. In figure 16a, simply increasing the Courant number by an order of magnitude does not necessarily mean an order of magnitude speedup. There is an interplay between the Courant number and the sparsity of the matrix. As the Courant number increase for the Markov matrix larger steps forward in time can be accurately calculated, but more operations are needed to calculate the next step in time. Overall, the Markov method for large Courant numbers with sparse matrix implementation is much faster than the PDE method and is faster than the previous implementation by C. Chen et al. [27]. It is expected that the Markov method should result in anywhere from 1 to 2 orders of magnitude speedup for a given problem, and could be even faster if implemented in a compiled programming language (like C++ or Fortran).

4 DISCUSSION

In this paper Markov methods for contaminant transport are extended to Courant numbers much larger than 1.0, as well as for transient source terms (under Courant numbers greater than 1.0), along with applications involving time varying flow fields. Although these methods show excellent speed increases from the standard PDE approaches, the initial overhead costs of calculating the Markov matrices can be computationally expensive. In order to construct a Markov matrix, \( n + n_{\text{source}} \) PDE simulations need to be computed. Access to high performance computing resources may be crucial for efficient calculation of these Markov matrices. However, once calculated, they can be easily stored and transferred for multiple applications. We envision very fruitful utilization of Markov methods for problems/applications that need very quick estimates of where contaminants may be at a time far in the future, or applications that allow these matrices to be used more than once, or cases where the information contained in the Markov matrix

5 The 5.59 times speedup reported in this previous study [27] was reported to be roughly independent of the number of elements in the discretization of the domain.
is further exploited. Some examples applications would be determining evacuation strategies once a toxic gas is dispersed somewhere in a building or building zone, using the matrices for demand response and control of the HVAC system, or using the matrices to determine sensor locations or quantify mechanical ventilation performance. With Markov matrices already showing applications with determining optimal sensor placement strategies and quantifying mechanical system ventilation performance, the methods developed in this paper allow for analysis in the applications for time varying flow fields. The methods are easily extendible to stochastic systems and problems with probabilistic boundary conditions (which is the focus of our future work). Other future directions include extracting more information from the Markov matrices themselves to create estimators for sensors, and identify contaminant source locations.

5 CONCLUSION

With a large number of potential harmful gases and particulates that the human body can be exposed to within indoor environments, it is important to have fast and accurate predictive numerical methods to determine concentrations within the indoor environment. While Markov based methods have been shown to be very efficient for this purpose, construction of these Markov matrices was problematic. In this paper, we develop two methods -- Eulerian and multistep Markov methods -- for the construction of Markov matrices with large Courant numbers (i.e. large time step sizes). We show that these methods result in Markov matrices that can be used to provide accurate scalar transport propagation (equivalent to traditional PDE methods), but at much higher Courant numbers. The methods developed can also include transient inlet and volumetric contaminant sources at large Courant numbers as well as be deployed for the calculation of contaminant transport under time varying flow fields. The ability to take large time steps (large Courant numbers) along with sparse implementation of the Markov matrices allowed for large speed increases -- from 30 times to 120 times faster than current state-of-art PDE based methods – for contaminant transport. We envision that Markov based methods can be very useful for real-time analysis and control of the indoor built environment.

NOMENCLATURE

\(Co\) The Courant number
\(D\) Contaminant diffusivity in air
\(f_{s,i}(x)\) The spatially varying function of the ith source term in the set of all contaminant sources
\(g_{s,i}(t)\) The time varying function of the ith source term in the set of all contaminant sources
\(g_{s,in}\) The time varying function of the inlet source
\(L(\cdot)\) The Perron-Frobenius operator
\(m\) The number of time instances between the starting time and \(\tau\)
\(n\) The number of cells or states in the domain
\(nb\) The number of boundary patches
\(n_{inlet}\) The number of inlet contaminant sources
\(n_{source}\) The number of sources terms
\(n_{vol}\) the number of volumetric contaminant sources
\(P\) Markov matrix
\(P(i,j)\) The i-th row and j-th column entry of the Markov matrix.
\(P(i,i+1)\) Markov matrix that propagates the scalar from time instant \(i\) to time instant \(i+1\)
\(P(t)\) The set of time varying Markov matrices used to propagate a scalar from time
instant 0 to time instant m

\( S \)  
Spatially continuous contaminant source

\( S_{(i,i+1)} \)  
Discrete contaminant source between the i-th and i+1 time instants

\( \hat{S}_{(0,i)} \)  
The effective source term from the zero-th time instant to the i-th time instant

\( \hat{S} \)  
The set of all contaminant sources

\( \hat{S}_i \)  
The i-th source term in the set of all contaminant sources

\( Re \)  
Reynolds number

\( T_{inlet} \)  
Temperature at the inlet

\( t \)  
time

\( t_{(i)} \)  
The i-th time instant

\( t_{PDE} \)  
The wall time required to complete a simulation with the PDE method

\( t_{Markov} \)  
The wall time required to complete a simulation with the Markov method

\( U \)  
Steady state velocity field

\( U_t \)  
Time varying velocity field

\( U \)  
Air speed in the domain

\( U_{in} \)  
Air speed at the inlet

\( U_{(i)} \)  
The velocity field at the i-th time instant

\( V_{ok} \)  
The volume of the k-th state

\( x \)  
The x-direction

\( y \)  
The y-direction

\( z \)  
The z-direction

\( \Delta t_{(i,i+1)} \)  
The times step between the i-th and the (i+1)-th time instant

\( \Gamma \)  
The set of boundary patches in the domain

\( \Gamma_{in} \)  
The set of inlet boundary patches

\( \Gamma_{out} \)  
The set of outlet boundary patches

\( \Gamma_w \)  
The set of wall boundary patches

\( \phi \)  
Continuous contaminant scalar field

\( \psi_{(i)}(k) \)  
Discrete contaminant concentration of state k at the ith time instant.

\( \psi_{in} \)  
Discrete contaminant concentration at the inlet

\( \psi_{(i)} \)  
The discrete contaminant concentration field at the i-th time instant

\( \tau \)  
Time interval for which the contaminant is spreading in the domain

\( \theta \)  
Normalized temperature

\( \omega \)  
a set of cells or stats in the domain

\( \Omega \)  
Domain of interest

REFERENCES


